
MAX IV

New Science at BioMAX and MicroMAX

Thomas Ursby
MAX IV Laboratory

MAX IV Laboratory

Short Pulse Facility
<100 fs pulses

1.5 GeV ring
96 m circumference,
DBA, 6 nm·rad

Linear accelerator
250 m long

Electron sources

3 GeV ring
528 m circumference,
MBA, 330 pm·rad

Beamline

The light that is produced by the electrons shines through the beamline to the experimental station. In the beamline one can choose which colour (wavelength) of the light to use and focus it on the sample to analyze. Some of the beamlines will need to be longer to reach higher performance.

Experimental stations

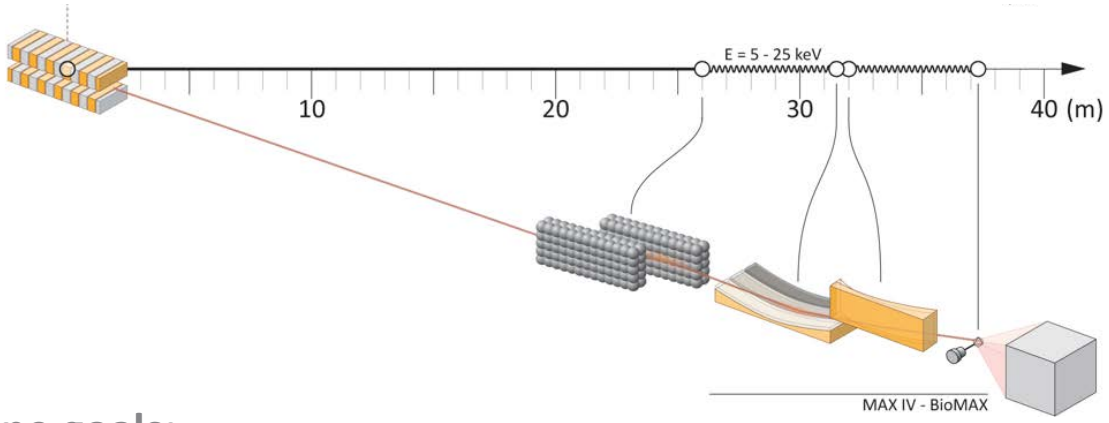
At the end of the beamline sits the experimental station. Each station is specialised to a specific science area. Here the samples is mounted and one measures what happens is illuminated by synchrotron radia-

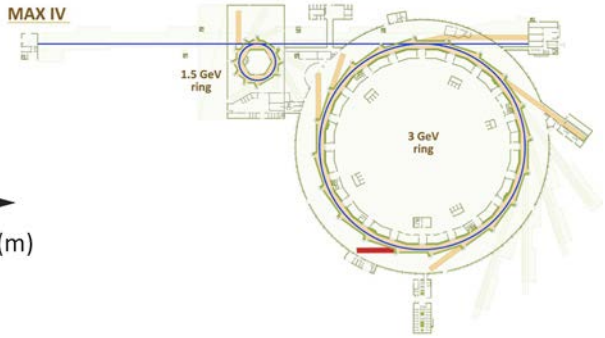
Radiation

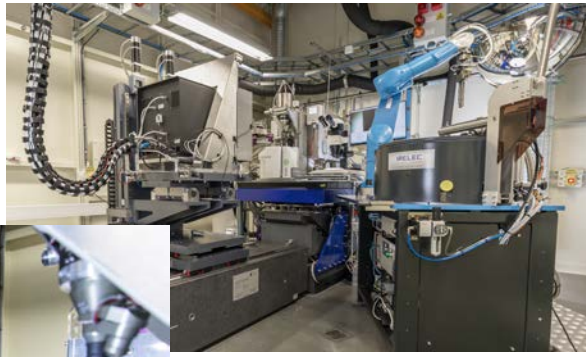
The electrons in the accelerator create a small amount of backgro
when the machine is operated. When the machine is switched off
maining radiation as no radioactive material is produced. The acc
is built into concrete and thus one can work freely in all other area
ratory. If someone would enter the accelerator area the machine
matically.

BioMAX – Macromolecular crystallography

BioMAX







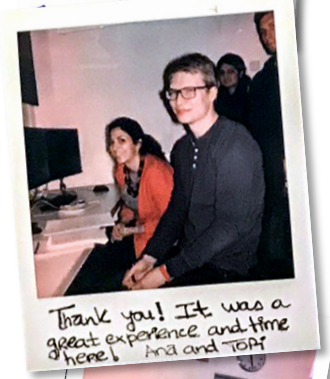
Beamline goals:

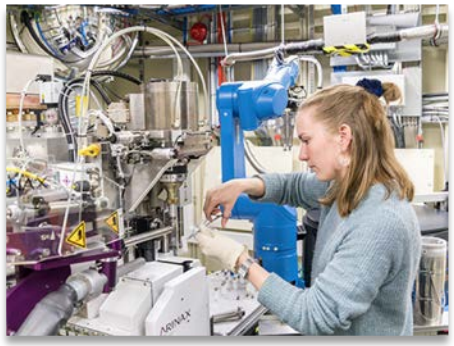
- ***Support all relevant techniques for MX***
- Beam characteristics:
  - Small focus (**20 x 5 μm²** hxv FWHM)
  - Low divergence (**0.1 x 0.1 mrad²**)
  - High flux (**2x 10^{13} phot/s x 0.1% bw**)
- Ultra stable beam
- Large energy range (5-25 keV)
- Short data collection times / high throughput
- High degree of automation

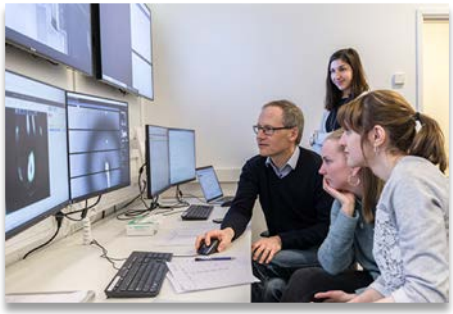
In regular user operation since 2017

Beamline Manager: Uwe Mueller

BioMAX user operation



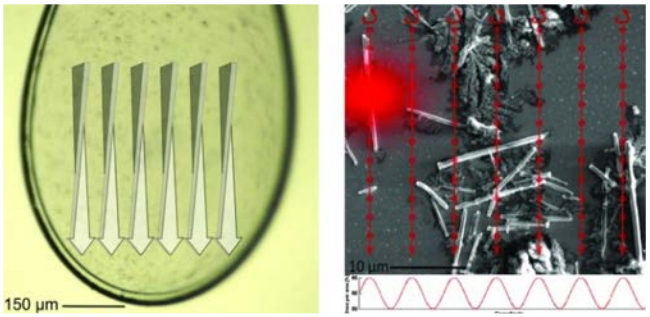




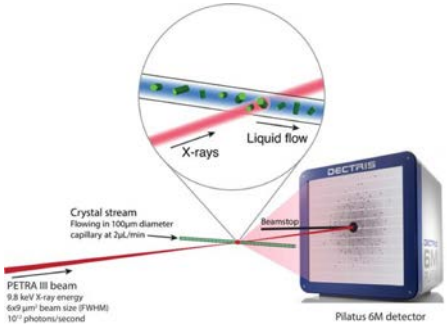
Serial Crystallography at BioMAX

Serial crystallography at synchrotron sources

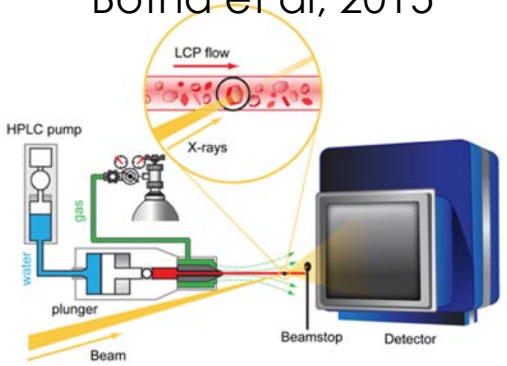
Cryogenic loop rotation
Gati et al. 2014



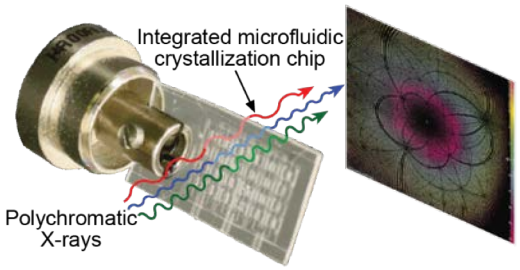
Glass capillary
Stellato et al., 2014



First injector-based experiments
Nogly et al., 2014
Botha et al, 2015



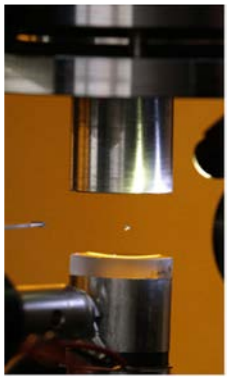
Fixed target systems



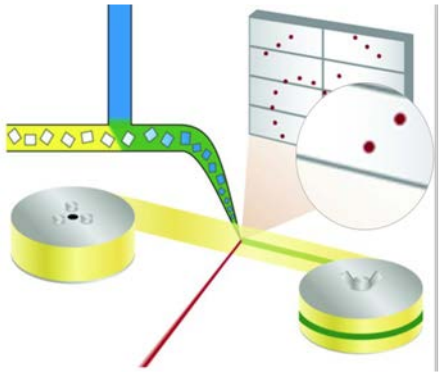
Silicon nitride membranes
Coquelle et al. 2015

Microfluidics chips
Sui et al., 2016

Ultrasonic acoustic levitation
S.Tsujino, T. Tomizaki, 2016



Moving tape
Beyerlein K. *et al.*, 2017



Serial Crystallography Sample Delivery

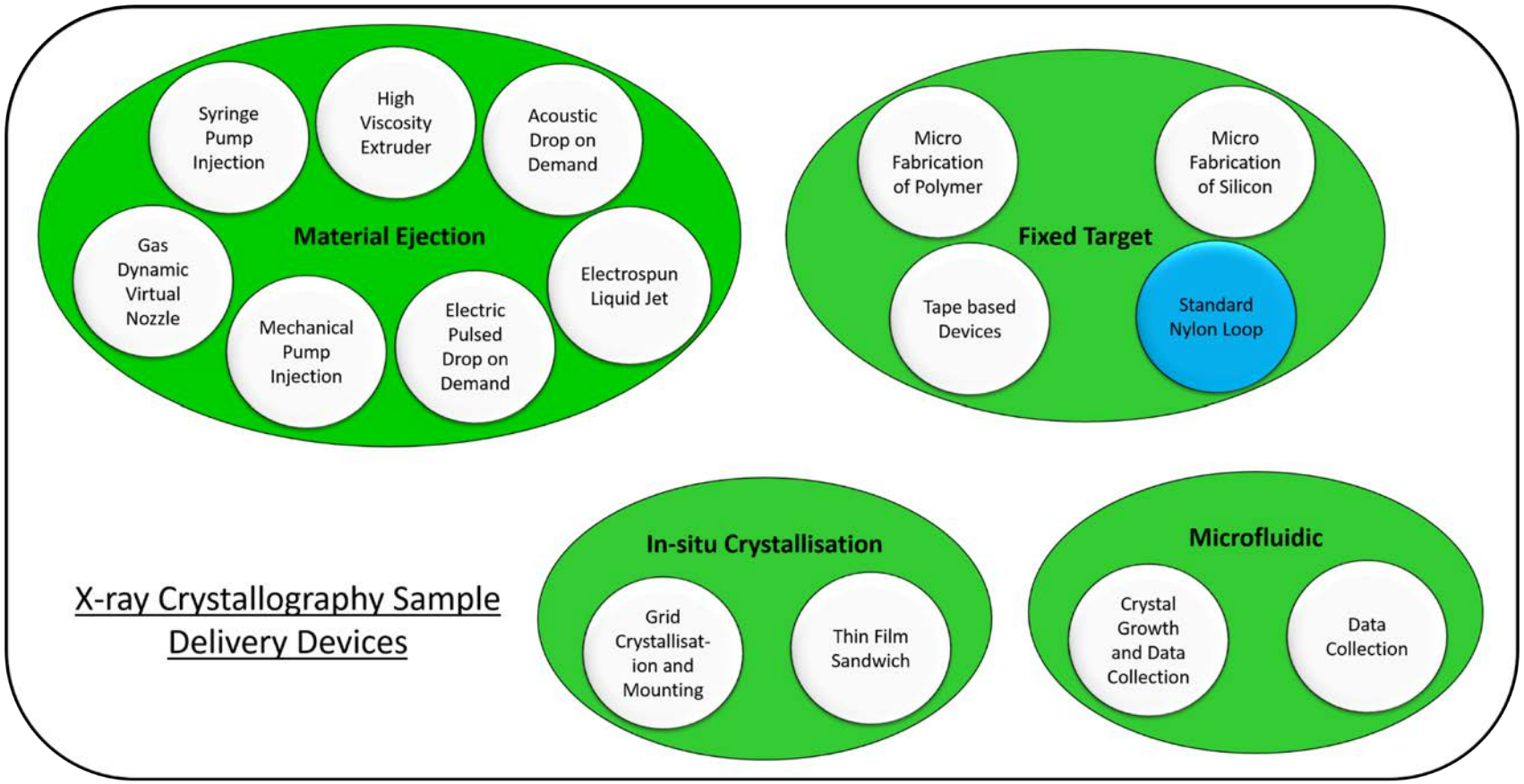
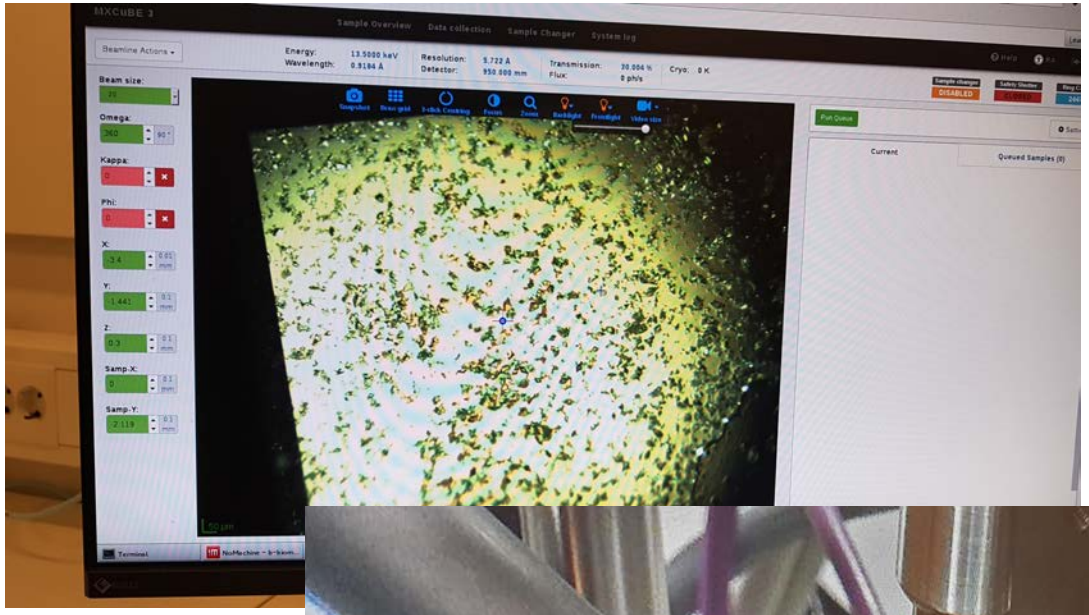
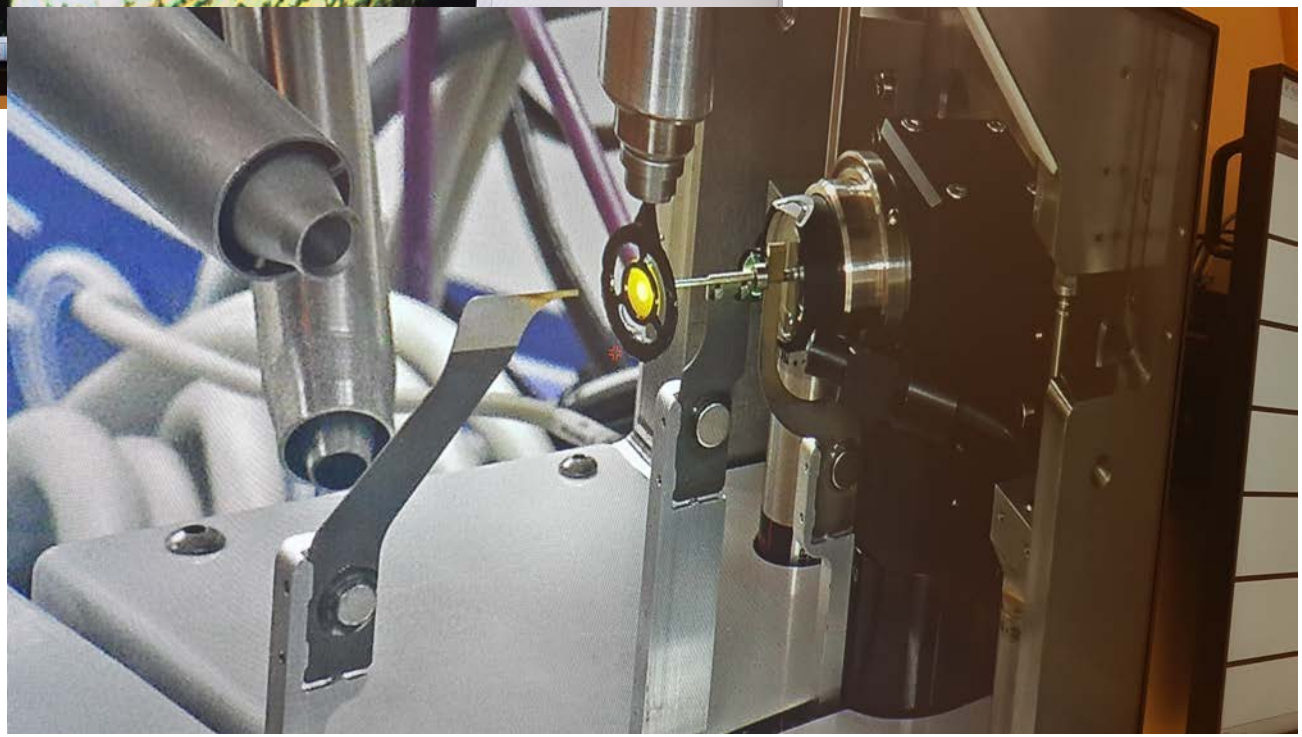


Figure Ross Friel

Overview X-ray Serial Crystallography Sample Deliver Devices

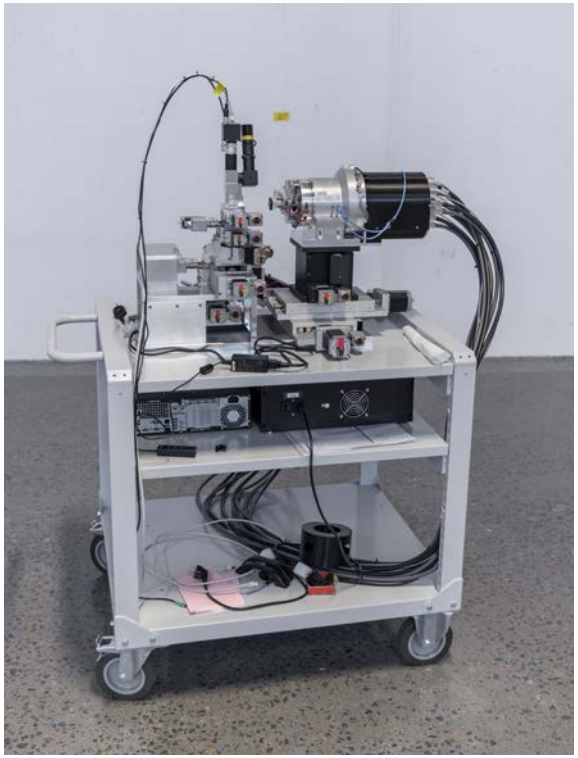
Fixed target using the MD3

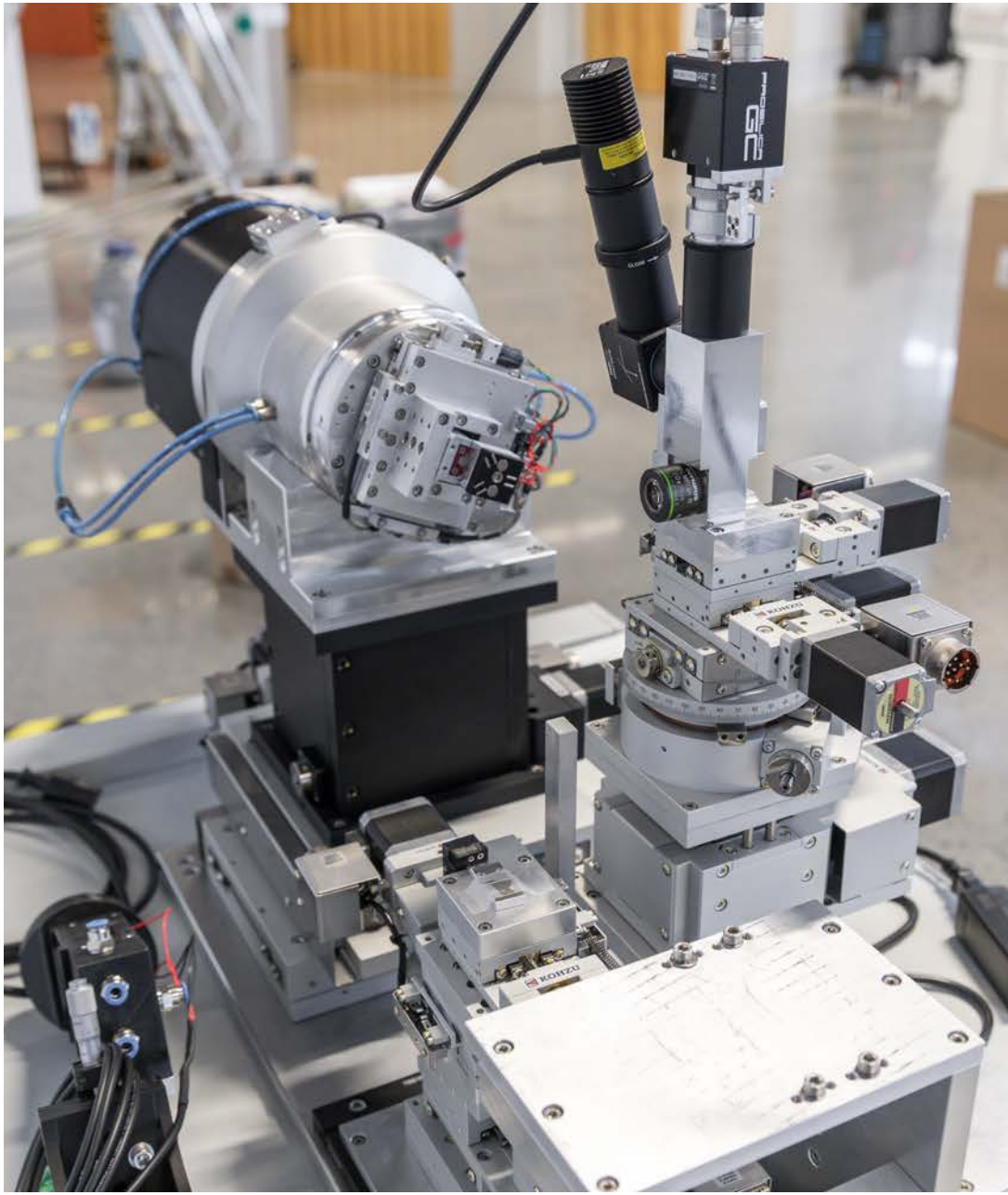




Fixed Target – Roadrunner

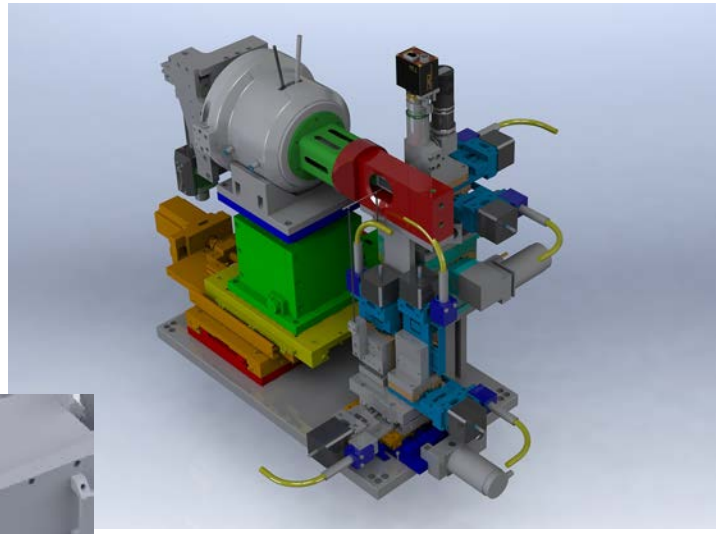
Alke Meents *et al.*, CFEL/DESY

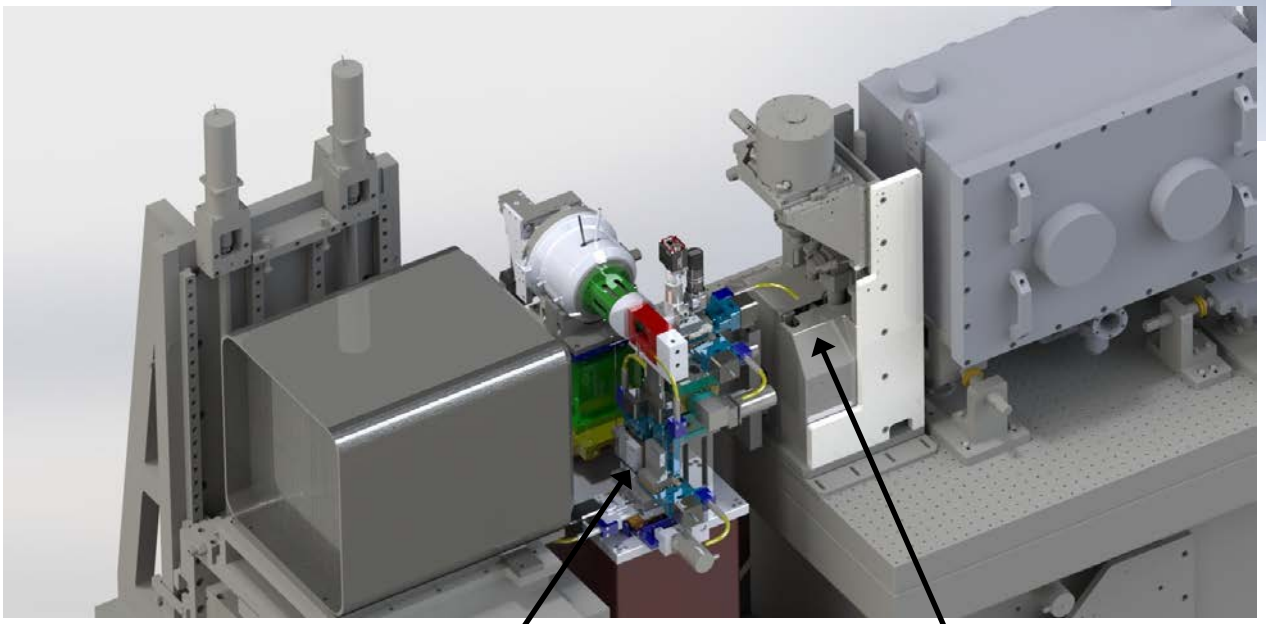




Fixed-target using Roadrunner

Roadrunner 3 at BioMAX, CAD view
In collaboration with Alke Meents CFEL/DESY





Roadrunner
scanning setup

MD3 diffractometer

High viscosity extrusion injector at BioMAX

Volume of the injector 130 µL

Pressurized via HPLC pump

Flow rate 1 µl per minute

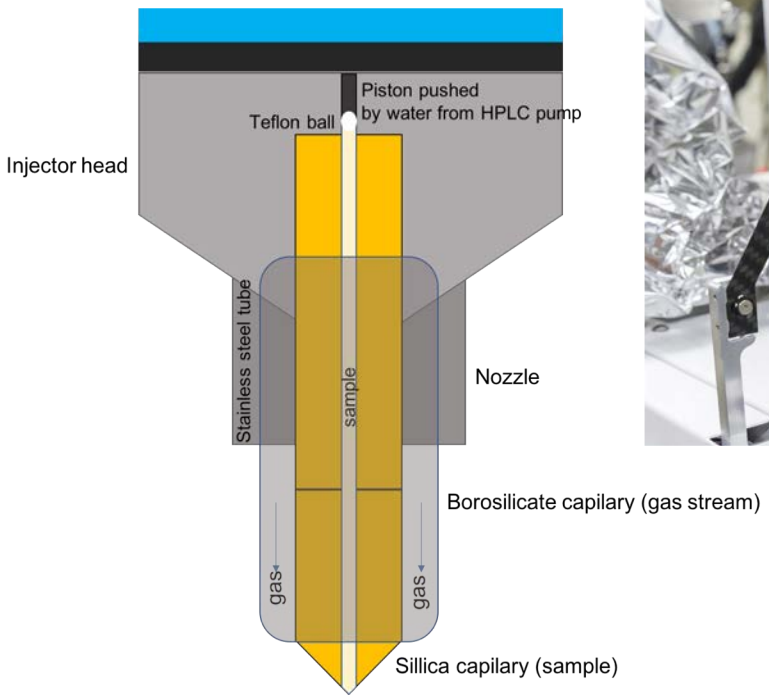
Exposure per crystal 2.8 ms

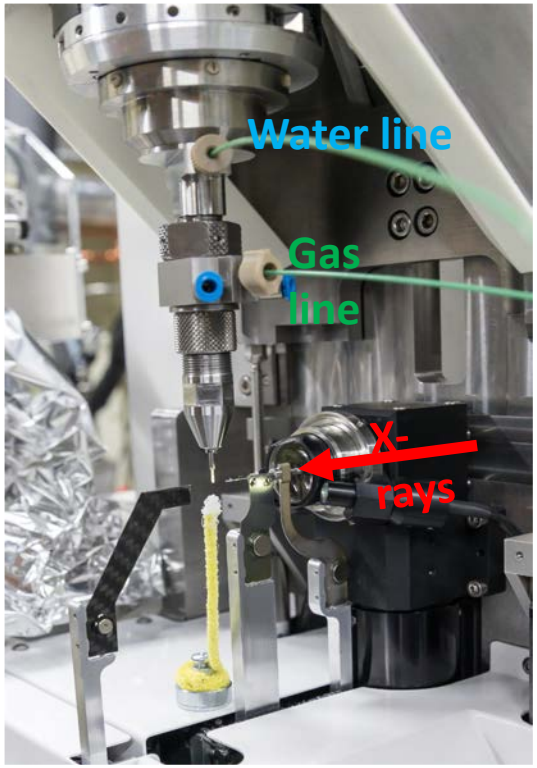
Frame rate 133 Hz

Low sample consumption

Different matrixes can be used

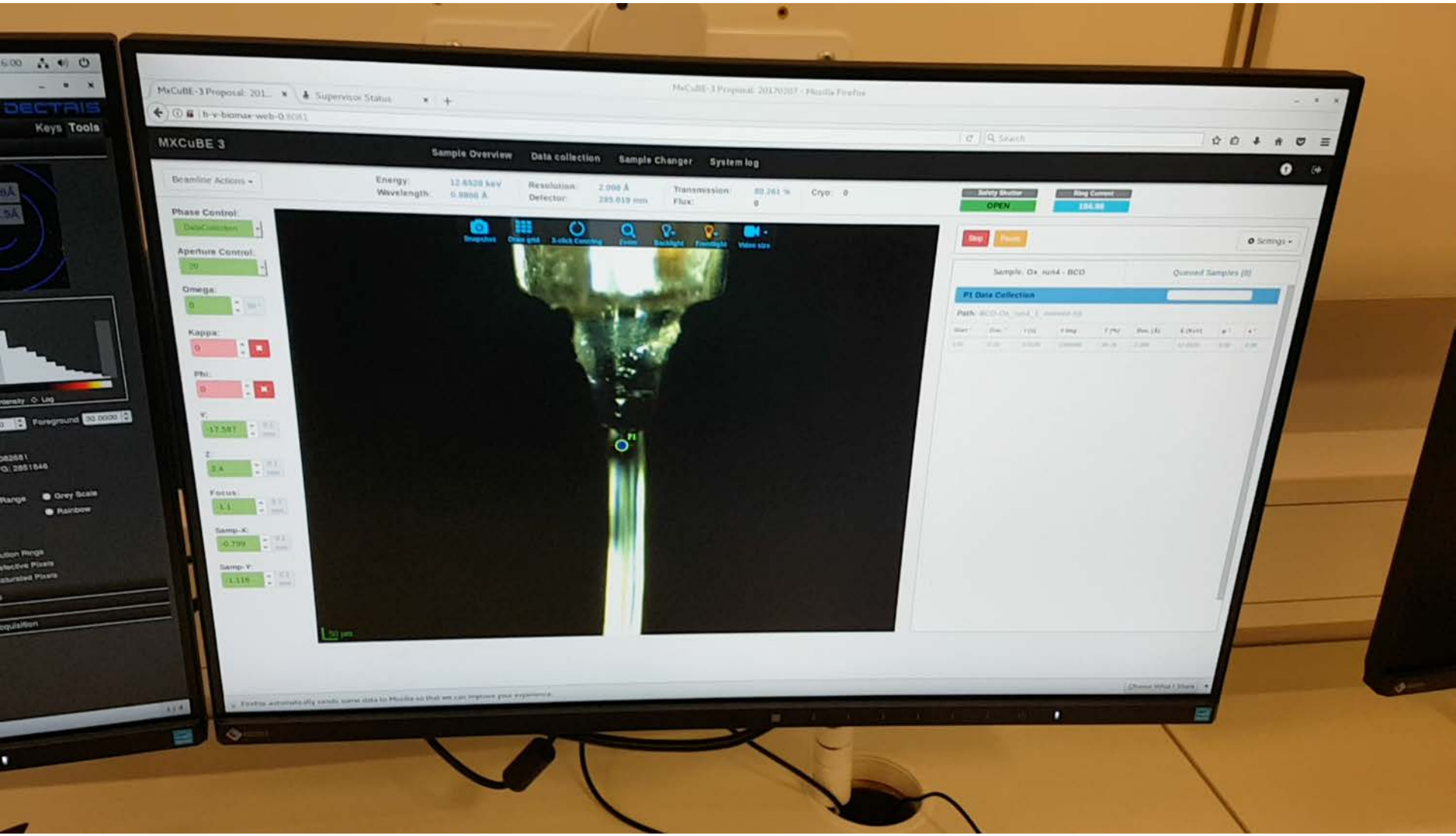
(grease, LCP, etc.)



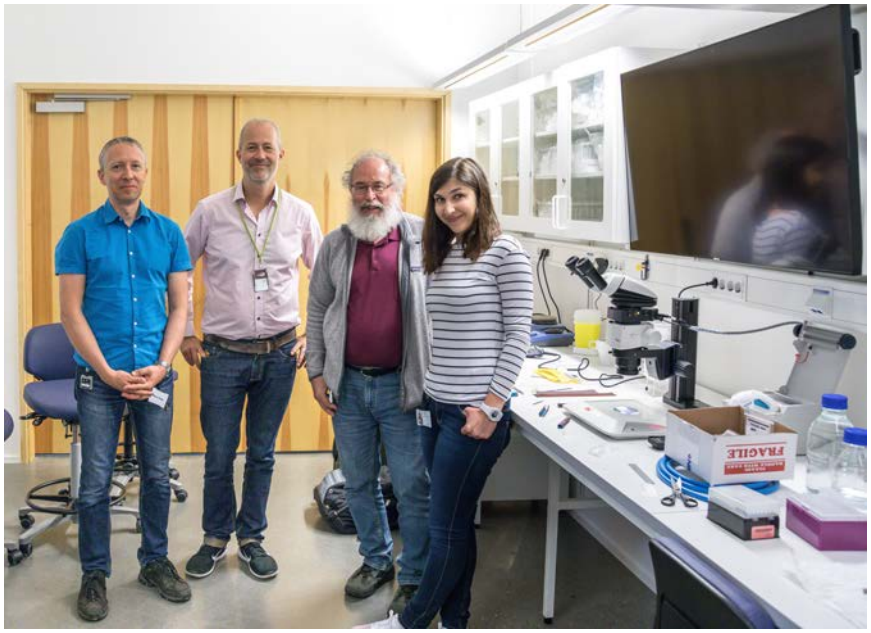


HVE injector developed at MPI Heidelberg
by Bruce Doak / Ilme Schlichting groups

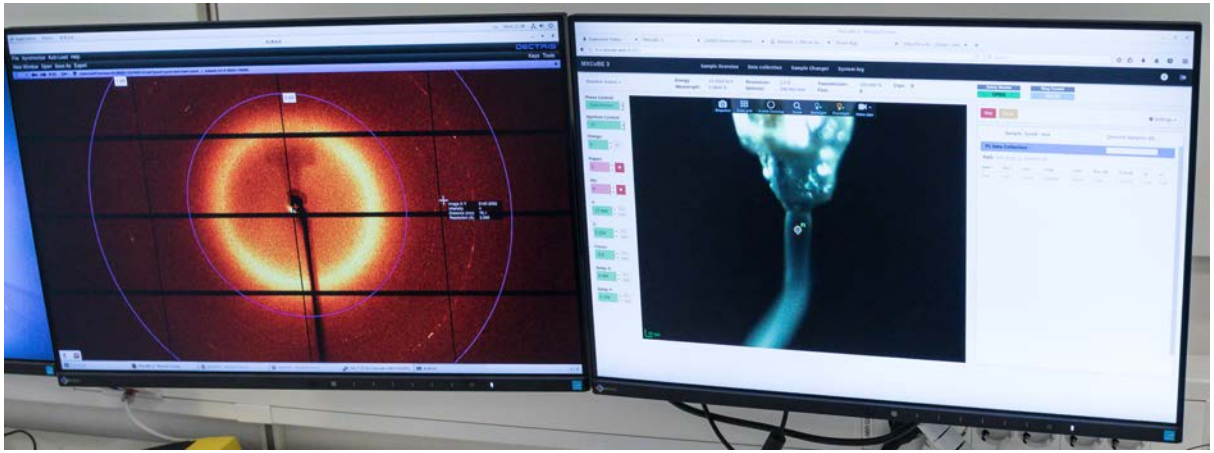
First HVE-injector experiment at BioMAX



First HVE-injector experiment at BioMAX



Robert Shoeman & Marco Kloos, MPI Heidelberg
Anastasya Shilova & Uwe Mueller, MAX IV



Data and extrusion viewer during experiment

First HVE-injector experiment at BioMAX

Average crystal size=10 µm

122,000 collected images

19,511 indexed images

Overall SNR = 4.8

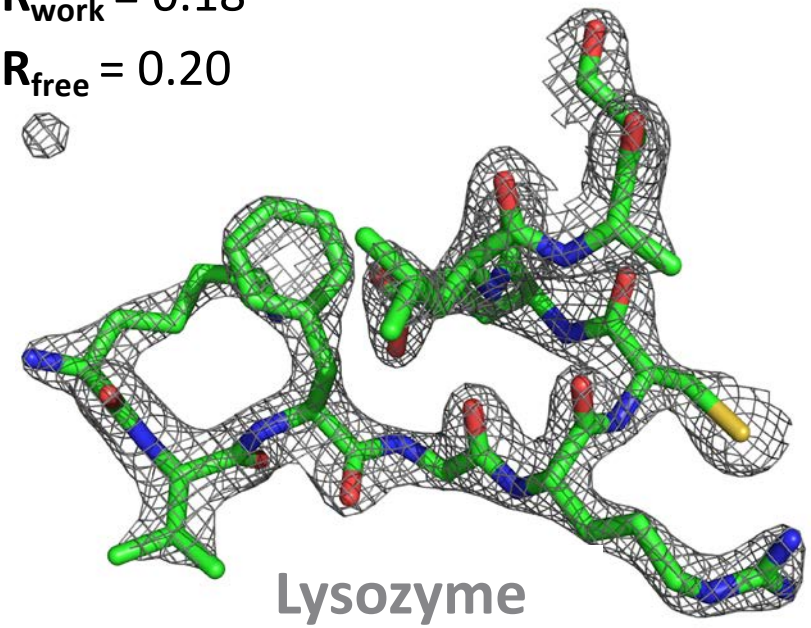
Completeness = 100%

Overall R_{split} = 14 %

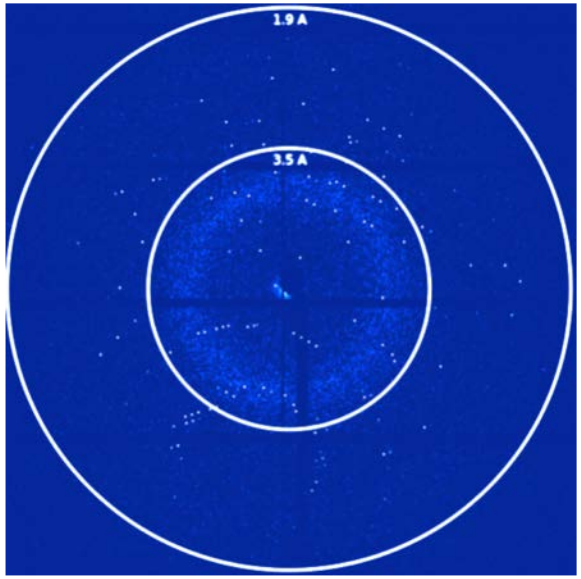
Resolution = 1.9 Å

R_{work} = 0.18

R_{free} = 0.20



Lysozyme



Sorting of data (NanoPeakCell)

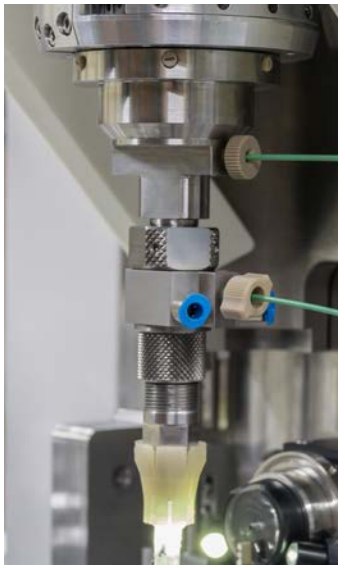
Merging and indexing of data (CrystFEL)

Phasing and refinement of data (Phenix, Coot)

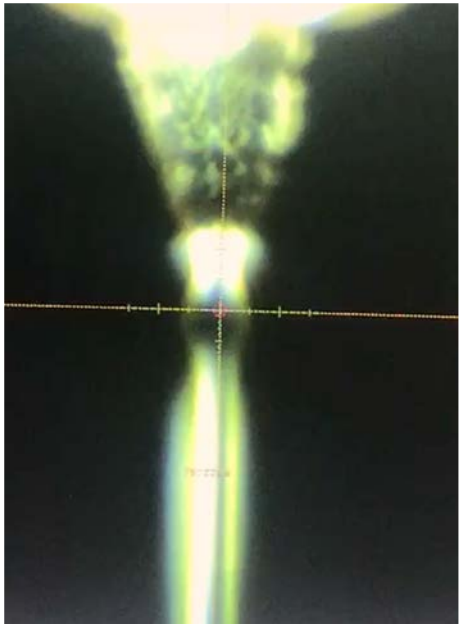
MAXIV

2nd HVE exp. – Neutze / Brändén groups

4 - 7 June 2018



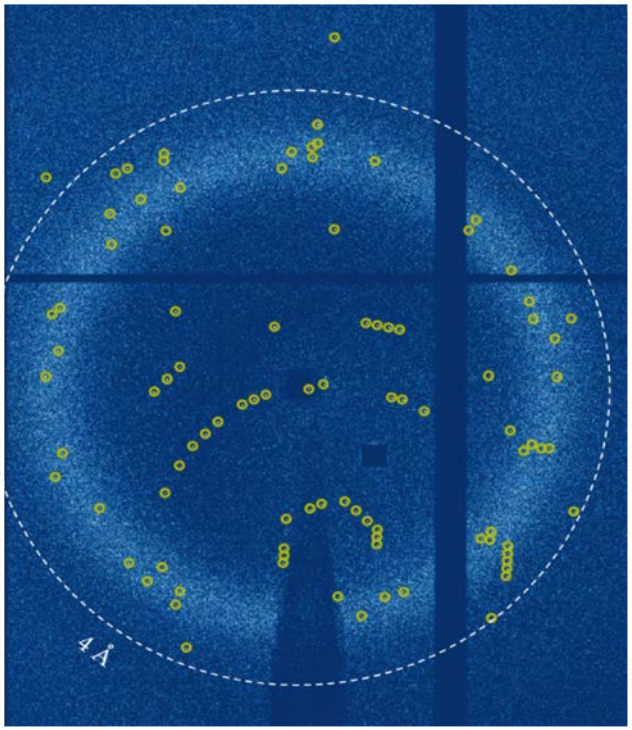
MPI HVE injector



- 3 projects injected
- 10 TB+ of data

First user HVE experiment at BioMAX

Average crystal size=15 µm
253,766 collected images
6,513 indexed images
Overall SNR = 2.7
Completeness=100%
Overall R_{split} = 34 %
Resolution = 3.8 Å
R_{work} = 0.32
R_{free} = 0.36



Cytochrome c oxidase enzyme

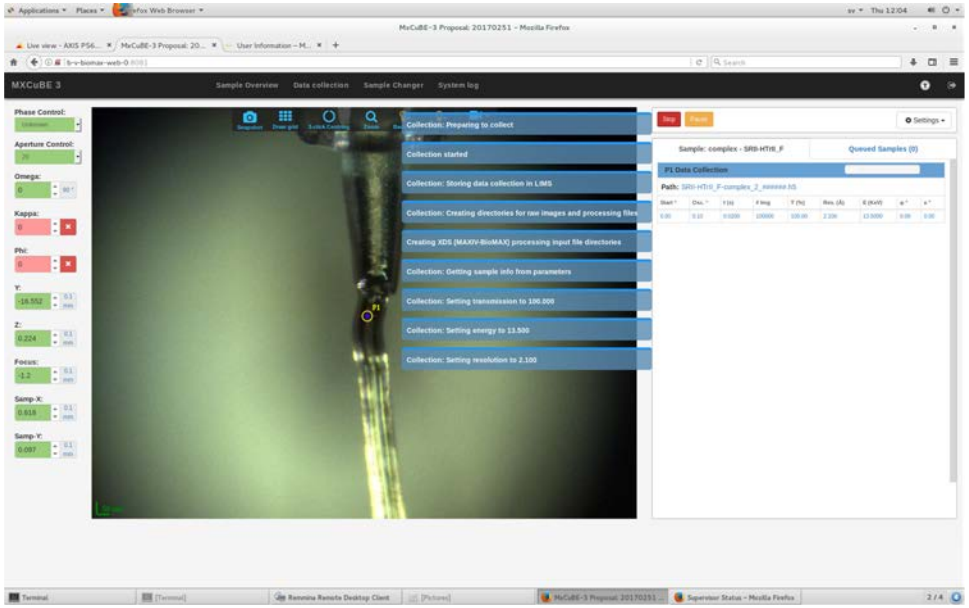
Experiment was performed with user groups from University of Gothenburg (groups of Richard Neutze and Gisela Brändén)

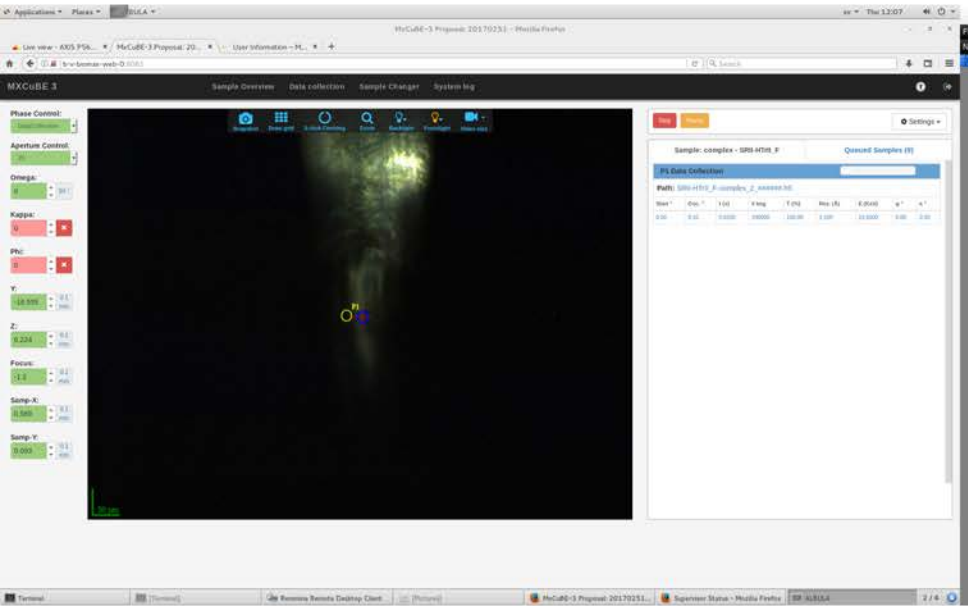
HVE injector experiments at BioMAX
Neutze / Brändén groups

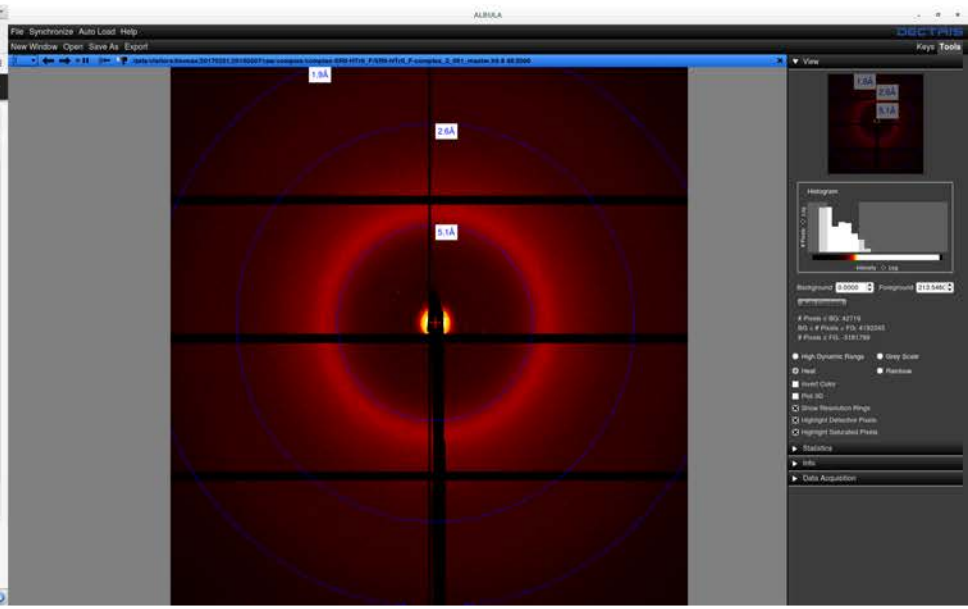
HVE injector experiments at BioMAX

MXCuBE

Separate branch (internal triggering of detector, 2D-centring and few other modifications)





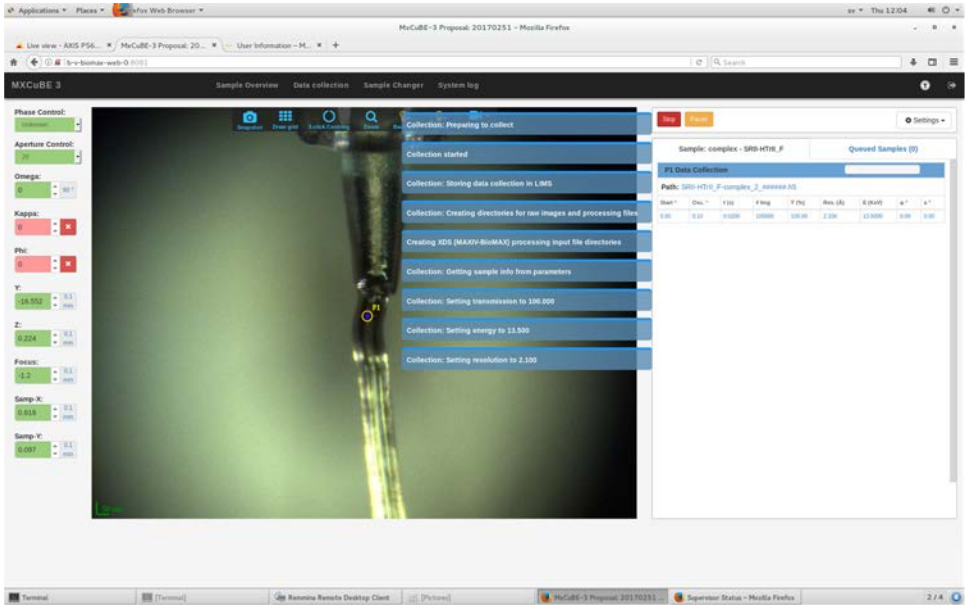


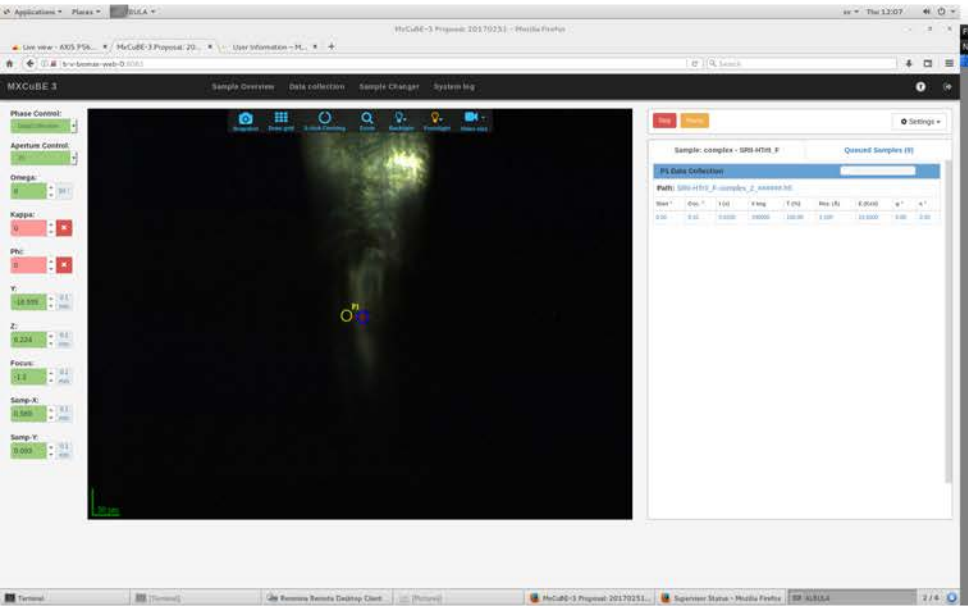
MXCuBE

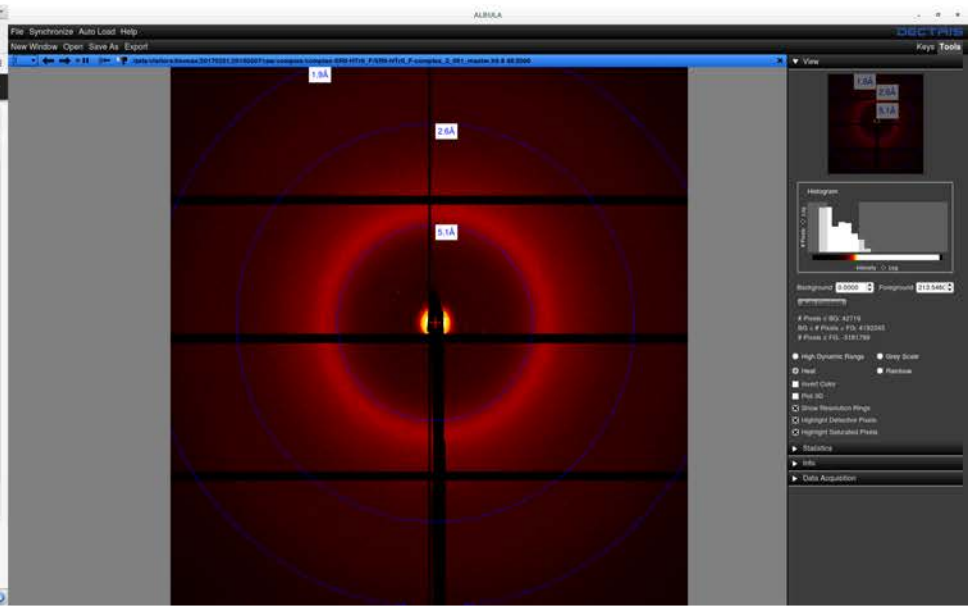
Improvements:

Add feedback of hit rate and processing statistics

A lot of small improvements could make the switch between oscillation and SSX experiments easier







Serial Crystallography at BioMAX

Bruce Doak, Ilme Schlichting *et al.*
Max Planck Institute for Medical Research, Heidelberg

Richard Neutze, Gisela Brändén *et al.*
University of Gothenburg

Alke Meents *et al.*, CFEL/DESY

Anastasya Shilova, Uwe Mueller, Jie Nan, Ross Friel,
Mirko Milas *et al.*
MAX IV MX Group

MicroMAX – Microfocus MX at MAX IV
MicroMAX – Serial Crystallography at MAX IV

MicroMAX Funding

The Novo Nordisk Foundation announced funding of MicroMAX on January 25th, 2018 (4 years of construction + 10 years of operation)

Beamlines

3.0 GeV Ring

NanoMAX
Nano-focus & coherence

DanMAX
Imaging & diffraction

Balder
EXAFS & RIXS

ForMAX
Wood based material

CoSAXS
SAXS & coherence

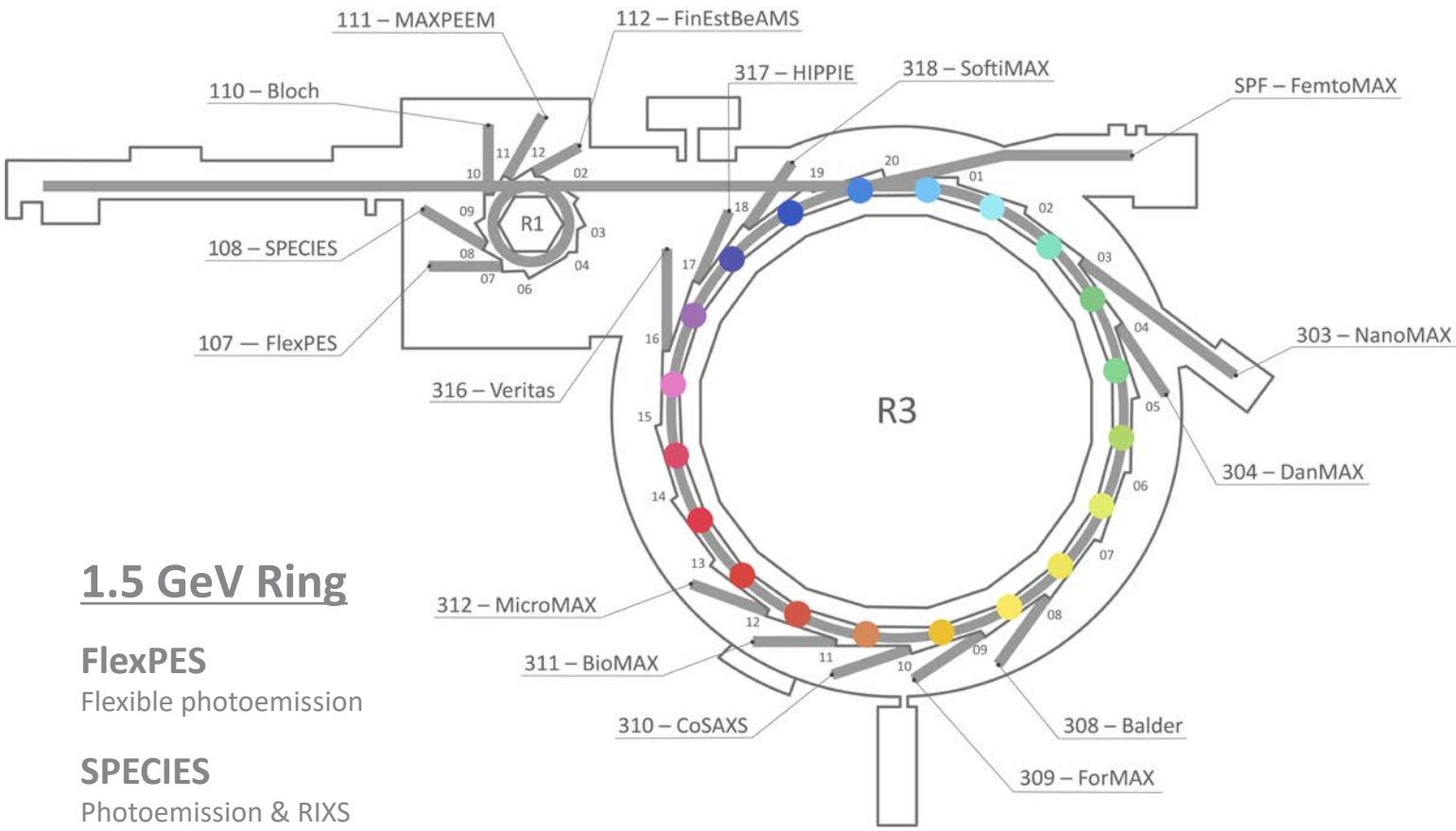
BioMAX
Protein structure

MicroMAX
Protein structure

Veritas
Excitations in solids & liquids

HIPPIE
Operando spectroscopy

SoftiMAX
X-ray microscopy & coherence



1.5 GeV Ring

FlexPES
Flexible photoemission

SPECIES
Photoemission & RIXS

Bloch
Electronic structure surfaces

MAXPEEM
Microscopy of surfaces

FinEstBeAMS
Gas phase & luminescence

3.0 GeV Linac

FemtoMAX
Ultra-fast diffraction & spectroscopy

Legend:
User operation
Commissioning
Construction

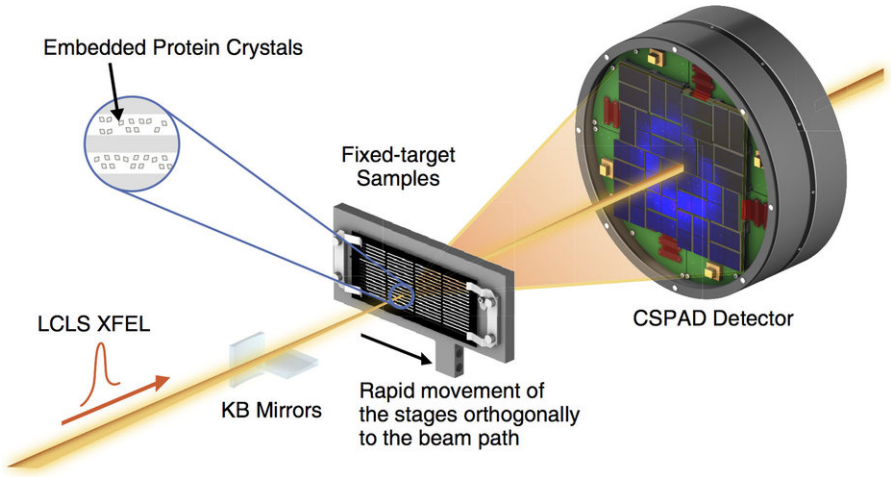
MAX IV

MicroMAX – Scope

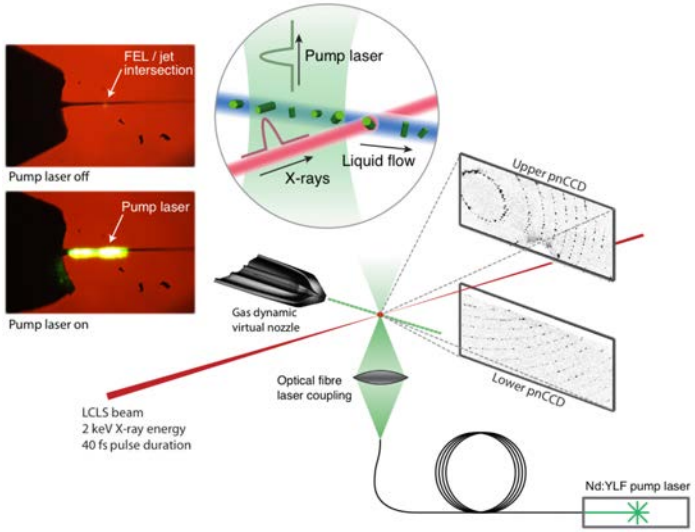
Study structure and function of macromolecules with a high brilliance X-ray beam and new beam delivery methods that will allow us to study:

- structures from macromolecules that cannot be crystallized to sufficient size or quality for other beamlines,
- room temperature structures,
- time resolved structures down to the micro- and millisecond timescales

A rapidly evolving field triggered by the development at XFELs

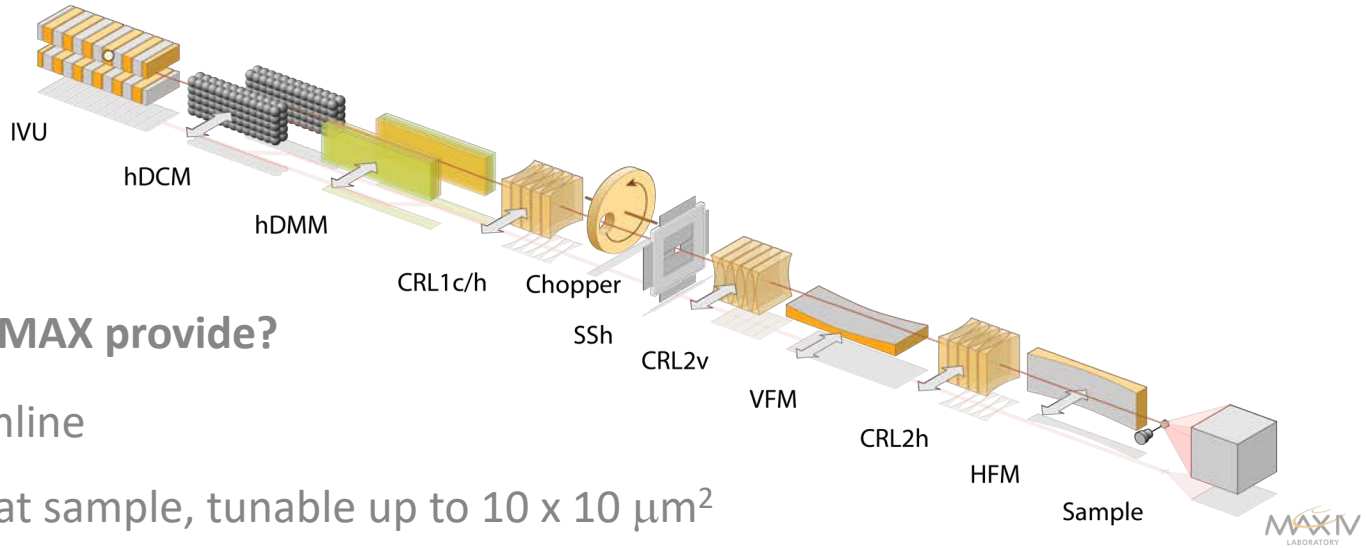


Hunter, M. S. et al. Fixed-target protein serial microcrystallography with an x-ray free electron laser. Sci. Rep. 4, (2014)



Aquila, A. et al. Time-resolved protein nanocrystallography using an X-ray free-electron laser. Opt. Express 20, 2706–2716 (2012)

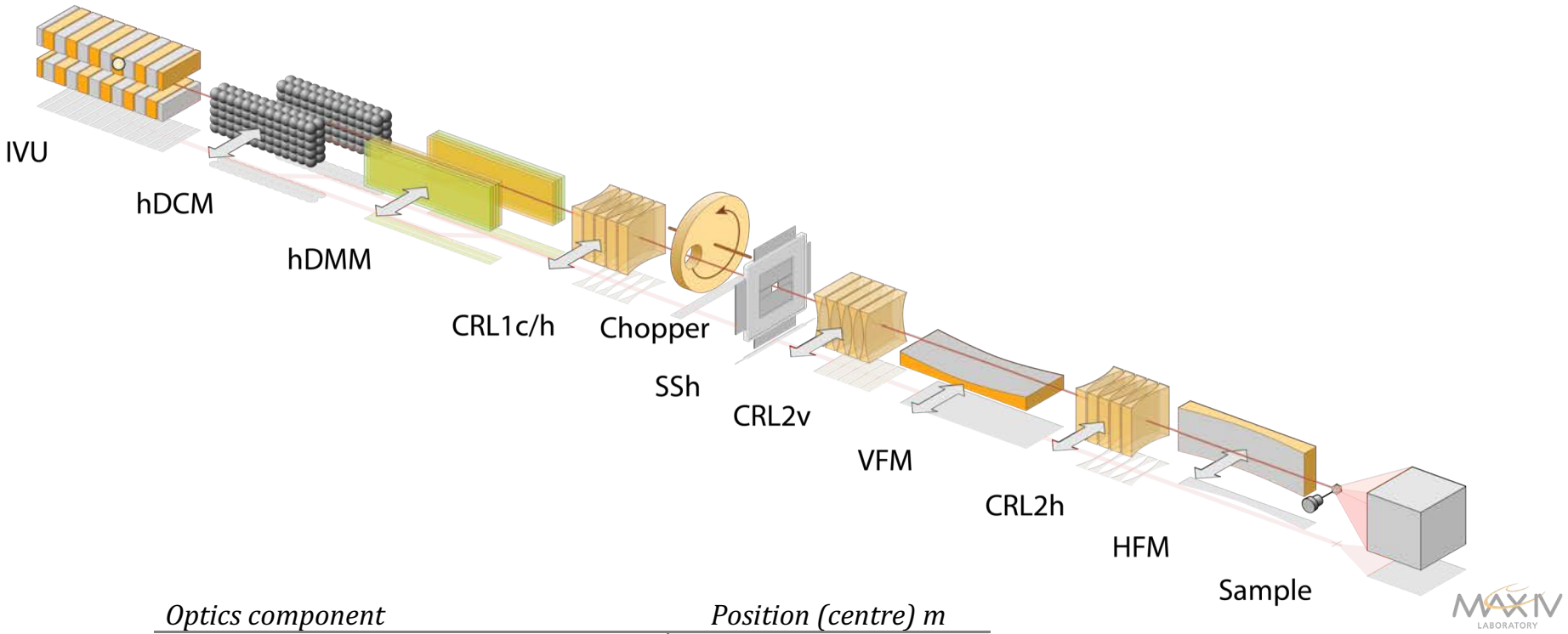
MicroMAX – Specifications



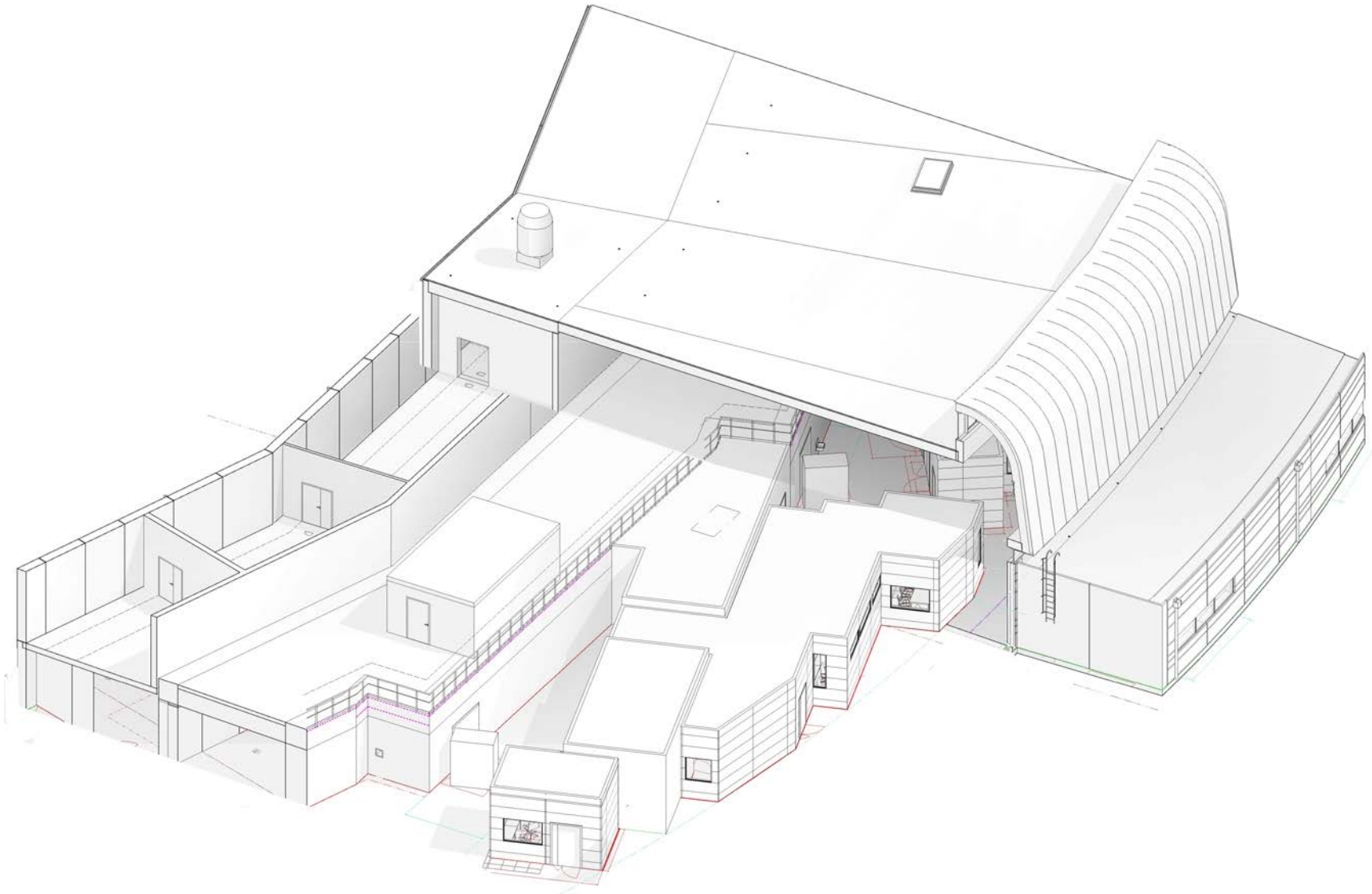
What should MicroMAX provide?

- Microfocus beamline
- 1 x 1 μm^2 beam at sample, tunable up to 10 x 10 μm^2
- Photon flux 10^{13} - 10^{15} photons/second (monochromatic / wider bandpass)
- Energy range 5 – 20 keV
- Exploratory setup (serial crystallography)
- Traditional setup (goniometry, sample environment)
- Optimal source for most demanding projects

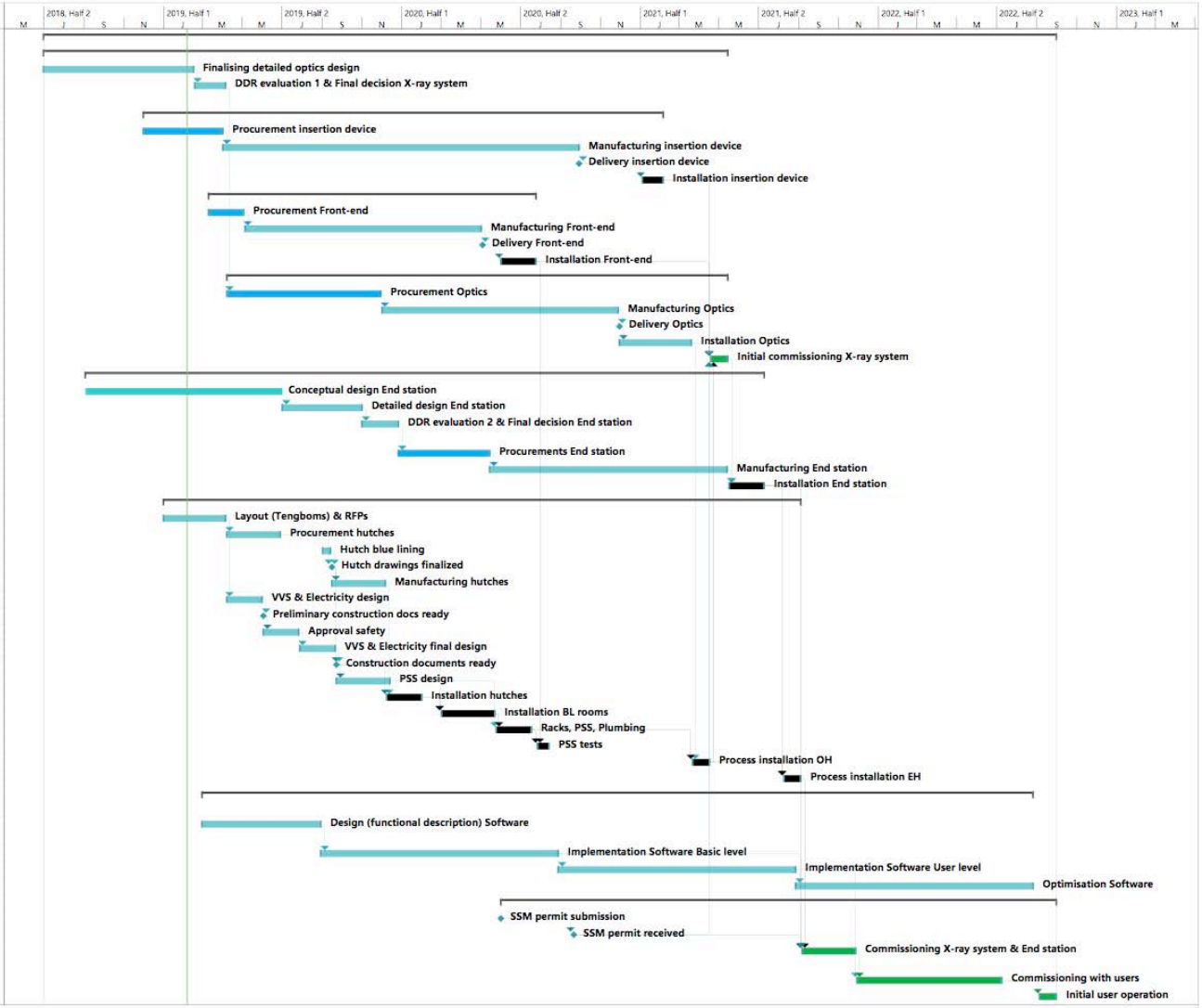
MicroMAX Optics



Optics component	*Position (centre) m*
In-vacuum undulator (IVU)	0
Crystal monochromator (hDCM)	24.7
Multilayer monochromator (hDMM)	25.5
Collimating lenses (CRL1c)	26.5
Horizontally focusing lenses (CRL1h)	26.9 ± 0.05
Chopper	32.0
Horizontal secondary source (SSh)	32.5
Vertically focusing lenses (CRL2v)	37.9 ± 0.1
Vertically focusing mirror (VFM)	38.4
Horizontally focusing lenses (CRL2h)	38.8 ± 0.03
Horizontally focusing mirror (HFM)	39.2
Diffractometer: Sample position EH1	40.0



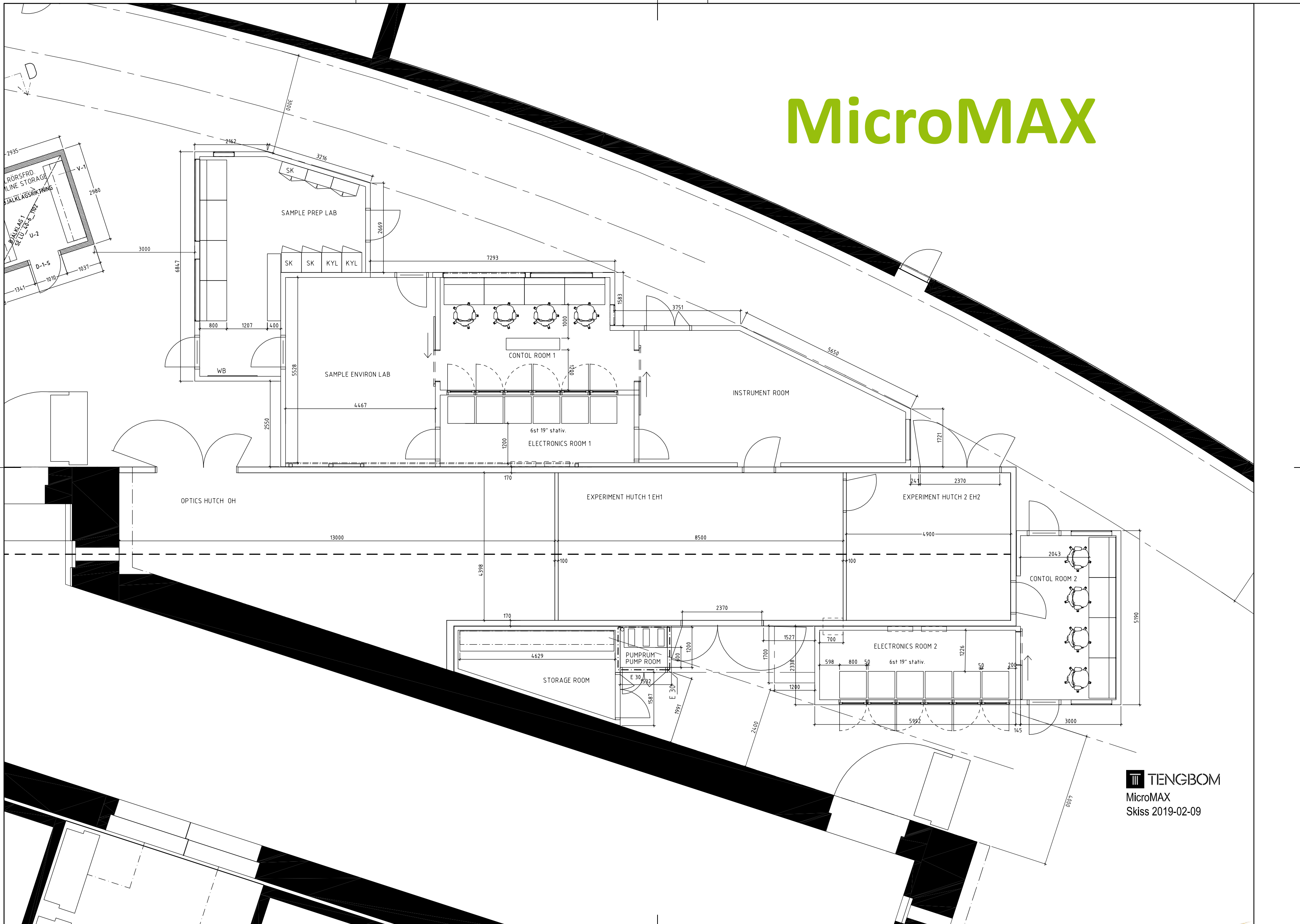
ID	Task Mode	Task Name	Duration	Start	Finish
1		**MicroMAX**	**1110 days**	**2018-07-01**	**2022-09-30**
2		**X-ray system**	**750 days**	**2018-07-01**	**2021-05-14**
3		Finalising detailed optics design	166 days	2018-07-01	2019-02-15
4		DDR evaluation 1 & Final decision X-ray system	35 days	2019-02-18	2019-04-05
5		**Insertion device**	**569 days**	**2018-12-01**	**2021-02-04**
6		Procurement insertion device	87 days	2018-12-01	2019-04-01
7		Manufacturing insertion device	78 wks	2019-04-02	2020-09-28
8		Delivery insertion device	0 days	2020-09-29	2020-09-29
9		Installation insertion device	24 days	2021-01-04	2021-02-04
10		**Front-end**	**360 days**	**2019-03-11**	**2020-07-24**
11		Procurement Front-end	8 wks	2019-03-11	2019-05-03
12		Manufacturing Front-end	52 wks	2019-05-06	2020-05-01
13		Delivery Front-end	0 wks	2020-05-04	2020-05-04
14		Installation Front-end	8 wks	2020-06-01	2020-07-24
15		**Optics**	**550 days**	**2019-04-08**	**2021-05-14**
16		Procurement Optics	34 wks	2019-04-08	2019-11-29
17		Manufacturing Optics	52 wks	2019-12-02	2020-11-27
18		Delivery Optics	0 days	2020-11-30	2020-11-30
19		Installation Optics	16 wks	2020-11-30	2021-03-19
20		Initial commissioning X-ray syste	4 wks	2021-04-19	2021-05-14
21		**End station**	**745 days**	**2018-09-03**	**2021-07-09**
22		Conceptual design End station	216 days	2018-09-03	2019-07-01
23		Detailed design End station	88 days	2019-07-02	2019-10-31
24		DDR evaluation 2 & Final decision End station	8 wks	2019-11-01	2019-12-26
25		Procurements End station	20 wks	2019-12-27	2020-05-14
26		Manufacturing End station	52 wks	2020-05-15	2021-05-13
27		Installation End station	8 wks	2021-05-17	2021-07-09
28		**Infrastructure & Safety**	**699 days**	**2019-01-01**	**2021-09-03**
29		Layout (Tengboms) & RFPs	69 days	2019-01-01	2019-04-05
30		Procurement hutches	12 wks	2019-04-08	2019-06-28
31		Hutch blue lining	2 wks	2019-09-02	2019-09-13
32		Hutch drawings finalized	0 days	2019-09-16	2019-09-16
33		Manufacturing hutches	12 wks	2019-09-16	2019-12-06
34		VVS & Electricity design	8 wks	2019-04-08	2019-05-31
35		Preliminary construction docs read	0 days	2019-06-03	2019-06-03
36		Approval safety	8 wks	2019-06-03	2019-07-26
37		VVS & Electricity final design	8 wks	2019-07-29	2019-09-20
38		Construction documents ready	0 days	2019-09-23	2019-09-23
39		PSS design	12 wks	2019-09-23	2019-12-13
40		Installation hutches	8 wks	2019-12-09	2020-01-31
41		Installation BL rooms	12 wks	2020-03-02	2020-05-22
42		Racks, PSS, Plumbing	8 wks	2020-05-25	2020-07-17
43		PSS tests	14 days	2020-07-27	2020-08-13
44		Process installation OH	4 wks	2021-03-22	2021-04-16
45		Process installation EH	4 wks	2021-08-09	2021-09-03
46		**Software (Control system and scientific computing)**	**910 days**	**2019-03-01**	**2022-08-25**
47		Design (functional description) Software	26 wks	2019-03-01	2019-08-29
48		Implementation Software Basic lev	52 wks	2019-08-30	2020-08-27
49		Implementation Software User lev	52 wks	2020-08-28	2021-08-26
50		Optimisation Software	52 wks	2021-08-27	2022-08-25
51		**Commissioning**	**610 days**	**2020-06-01**	**2022-09-30**
52		SSM permit submission	0 days	2020-06-01	2020-06-01
53		SSM permit received	0 days	2020-09-21	2020-09-21
54		Commissioning X-ray system & End station	12 wks	2021-09-06	2021-11-26
55		Commissioning with users	32 wks	2021-11-29	2022-07-08
56		Initial user operation	4 wks	2022-09-05	2022-09-30



Project: MicroMAX v2
Date: 2019-02-06

Task | Split | Milestone | Summary | Project Summary | Inactive Task | Inactive Milestone | Inactive Summary | Manual Task | Duration-only | Manual Summary Rollup | Manual Summary | Start-only | Finish-only | External Tasks | External Milestone | Deadline | Progress | Manual Progress

MicroMAX



TENGBOM
MicroMAX
Skiss 2019-02-09

MicroMAX

Open position:

Experiment station scientist

https://www.maxiv.lu.se/about-us/careerjobs/vacancies/

Application deadline March 24

Beamline/Experimental station scientist MicroMAX temporary (2 year)

Lunds universitet, MAX IV, MX group

Lund University was founded in 1666 and is repeatedly ranked among the world's top 100 universities. The University has 40 000 students and 7 400 staff based in Lund, Helsingborg and Malmö. We are united in our efforts to understand, explain and improve our world and the human condition.

MAX IV is a Swedish national large-scale research laboratory hosted by Lund University. It provides scientists from Sweden as well as internationally, with state-of-the-art instrumentation for research in areas such as engineering, physics, structural biology, chemistry and nanotechnology. Fully developed it will receive more than 2 000 scientists annually, conducting ground-breaking experiments in materials and life sciences using the brilliant X-ray light. As a national laboratory, MAX IV is operated in agreement with governmental regulations, and in compliance with major funders such as the Swedish Research Council (VR) and the Wallenberg Foundation. 250 people are currently employed at MAX IV Laboratory, and 16 beamlines are funded. The facility is in a ramp-up phase with 3 beamlines now receiving users and 13 more scheduled to be commissioned and built to receive users within the next few years. The facility is dimensioned for 25-28 beamlines.

MAX IV Laboratory recently received funding from the Novo Nordisk Foundation (http://novonordiskfonden.dk/en) for a new beamline called MicroMAX (https://www.maxiv.lu.se/micromax/), a micro-focus macromolecular crystallography beamline. MicroMAX will exploit new sample delivery methods and the unique performance of the MAX IV 3 GeV storage ring to provide new possibilities in collecting high quality structural data from microcrystals.

MicroMAX will build on the rapid development of serial crystallography that is presently attracting great interest within the structural biology community. MicroMAX will not only increase the probability of obtaining structural data from challenging projects where only microcrystals are available but also enable data collection at room temperature and time resolved experiments with a time resolution down to the microsecond range.

The Macromolecular Crystallography (MX) group is responsible for the BioMAX beamline that is in operation and the design, construction and future operation of the MicroMAX beamline. We have started developing activities in the field of serial crystallography and we have already performed experiments at BioMAX.

We are now looking for a beamline scientist to lead the design and construction of the experiment station. We foresee that a permanent position will be advertised in a later stage of the project to finalize the station, take it in user operation and to continue the technical and scientific developments.

Tasks

You will take a leading role in the design and construction of the MicroMAX experiment setup. You will work closely with the MicroMAX research engineer and project manager and other staff within the MicroMAX team and MX group. A major aspect of the experiment setup is the evaluation and implementation of different sample delivery systems that exist and that are being developed by us and the community. An important part of your work will be to create a flexible solution to accommodate these different sample delivery systems, and to incorporate and further develop the different sample delivery systems in collaboration with other members of the MX group and other external collaborating groups. Your work will involve interactions with other groups at MAX IV, collaborating groups and suppliers as well as handling of procurements and administrative tasks.

You will participate in the user support, especially with the already existing serial crystallography environments at BioMAX, and within the on-call service of BioMAX and later MicroMAX.

You are strongly encouraged to develop your own research project and collaborations. Furthermore, you will have to participate in experiments at MAX IV or at other facilities, in particular related to the use and development of serial crystallography or time-resolved crystallography.

Qualifications

Macromolecular Crystallography Group

Mikel Eguiraun
Ross Friel
Andrea Gross
Ana Gonzalez
Gustavo Lima
Mirko Milas
Jie Nan
Anastasya Shilova
Johan Unge
Thomas Ursby
Uwe Mueller

Funding MAX IV Facility

Vetenskapsrådet
Lunds Universitet
VINNOVA
Region Skåne
Lunds Universitet
Uppsala Universitet
KTH
Chalmers
Knut och Alice Wallenbergs Stiftelse
Luleå Tekniska Universitet
Karolinska Institutet
SLU
Göteborgs Universitet

MicroMAX funding: novo nordisk fonden

MAX IV

Thank you for your attention!